

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.25e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.49e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

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(2E)-3-Phenylprop-2-enal

Measured: 4.80e-11

Predicted: 5.31e-11

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(E)-Crotonaldehyde

Measured: 3.61e-11

Predicted: 3.73e-11

Image not found

Crotonaldehyde

Measured: 3.61e-11

Predicted: 3.73e-11

Image not found

Glyoxal

Measured: 1.14e-11

Predicted: 1.14e-11

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(2E)-2-Hexenal

Measured: 4.40e-11

Predicted: 4.31e-11